Calculation of the phase of hidden rotating antiferromagnetic order

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Abstract

The phase of the rotating order parameter in rotating antiferromagnetism is calculated using a combination of mean-field theory and Heisenberg equation. This phase shows a linear time dependence, which allows us to interpret rotating antiferromagnetism as a synchronized Larmor-like precession of all the spins in the system or as an unusual $\mathbf{q} = (\pi, \pi)$ spin-wave around a zero local magnetization. We discuss implications for the pseudogap state of high-T_C superconducting materials. Rotating antiferromagnetism has been proposed to model the pseudogap state in these materials.

Keywords: Hidden order, rotating antiferromagnetism, High-T_C cuprates, Pseudogap energy, phase of rotating order

1. Introduction

According to several researchers, the puzzling pseudogap (PG) phenomenon in high-T_C superconductors (HTSC) is caused by some sort of hidden order. This is supported by the observation of a depression in the density of states at the Fermi level, with no order parameter responsible for this depression observed yet [1, 2, 3, 4]. Rotating anti-ferromagnetism (RAF) has been recently proposed as a possible candidate for this hidden order, and several physical quantities have already been calculated within the RAF theory (RAFT) with good agreement with available experimental data [5, 6, 7]. RAF is one of several other proposals for the PG (see Ref. [4] for a discussion). Contrary to theories of circulating currents [8, 9, 10], RAF is based on the concept of an order parameter that has a finite magnitude below a critical temperature but a time-dependent phase [11]. Note that all the physical quantities that have so far been calculated within RAFT do not depend on the phase of the order parameter in RAF [5, 6, 7, 12, 13, 14, 15]. The lack of the time dependence profile for this phase limited however the full understanding of the nature of RAF. The purpose of this work is to calculate this phase as a function of time using a combination of RAFT and the Heisenberg equation. We show that it varies linearly with time. As a consequence of this time dependence, RAF can be interpreted as a (π, π) unusual spin wave around a zero local magnetization or as a synchronized Larmor-like precession of all the spins in the system. Because the phase of this order parameter is time dependent, it was not possible to calculate it in RAFT alone, which is a mean-field approach.

This paper is organized as follows. First in Sec. 2.1 we rederive RAFT using the spin ladder operators, which are necessary for the phase calculation. In Sec. 2.2, we review RAFT. Then in Sec. 2.3 we use the Heisenberg equation to get the time dependence for the spin ladder operators, which yields the time dependence of the phase of the rotating order parameter. In Sec. 2.4, the interpretation of RAF as an unusual (π, π) spin wave is explained. Finally, conclusions are drawn in Sec. 3.

2. Approach

As we are only interested in understanding the nature of the PG phase of HTSCs in this work, we restrict ourselves to the non superconducting phase. Consider the *t-t′* Hubbard model in two dimensions:

$$H \quad = \quad -t \sum_{\langle i,j \rangle \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.}$$

$$-\mu \sum_{i,\sigma} n_{i,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $\langle i, j \rangle$ and $\langle\langle i, j \rangle\rangle$ designate summation over nearest and second-nearest neighboring sites, respectively. t and t' are electron hopping energies to nearest and second-nearest neighbors, respectively. Because the phase of RAF is related to the spin ladder operators, it is useful to rewrite Hamiltonian (1) using these operators.

2.1. Rewriting the Hamiltonian using the spin ladder operators

Using the spin ladder operator written in second quantization $S_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow}$, the onsite Coulomb repulsion term $U n_{i\uparrow} n_{i\downarrow}$ can on one hand be cast in the form $U n_{i\uparrow} n_{i\downarrow} = U n_{i\uparrow} - U S_i^+ S_i^-$ and on the other hand as $U n_{i\uparrow} n_{i\downarrow} = U n_{i\downarrow} - U S_i^- S_i^+$. Summing and dividing by 2 yields the symmetrized expression $U n_{i\uparrow} n_{i\downarrow} = \frac{U}{2}(n_{i\uparrow} + n_{i\downarrow}) - \frac{U}{2}(S_i^+ S_i^- + S_i^- S_i^+)$. The latter can be proved by calculating the action of each side of the equality on the possible states $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$, and noting that $S_i^+ S_i^- |\uparrow\downarrow\rangle = S_i^- S_i^+ |\uparrow\downarrow\rangle = 0$ due to Pauli exclusion principle, and $S_i^+|0\rangle \equiv c_{i\uparrow}^\dagger c_{i\downarrow}|0\rangle = 0$. For our many-body system, sites are neither full nor empty, but are on average occupied by a density smaller than 1 away from half filling. Therefore, the terms $S_i^+ S_i^-$ and $S_i^- S_i^+$, which are responsible for onsite spin-flip excitations, will contribute by lowering energy for the sites that are partially occupied by the same density of spin up and down electrons. One can decouple this term in mean-field theory using $\langle S_i^- \rangle \equiv \langle c_{i,\downarrow}^\dagger c_{i,\uparrow} \rangle$, which leads to a collective behavior for the spin-flips, and the results obtained in this way are the same as in RAFT [5, 6, 7, 12, 13, 14]. In this state, a spin flip process at site i is simultaneously accompanied by another one at another site j; the occurrence of the spin flips is synchronized. Thermal motion has obviously an effect on this order as it does on conventional orders; i.e., above a critical temperature (identified with the PG temperature) the spin-flip processes become uncorrelated, leading to the disappearance of the long-range non conventional order. The spin-flip processes, which are purely quantum, continue to exist even above this critical temperature, but in an incoherent disordered manner. The occurrence in RAFT of a second-order phase transition at the PG temperature is consistent with experimental data supporting its existence [4].

2.2. Review of RAFT

We rederive RAFT, which deals with the static part (magnitude) of the order parameter $\langle S_i^\pm \rangle$, using the spin ladder operators then for the dynamic (phase) part we will use the Heisenberg equation to find its time dependence. To the best of our knowledge the combination of mean-field theory and the Heisenberg equation of quantum mechanics constitutes a novel approach for the PG in HTSCs.

The parameter $Q_i = \langle c_{i,\uparrow} c_{i,\downarrow}^\dagger \rangle = -\langle S_i^- \rangle \equiv |Q|e^{i\phi_i}$ is defined in order to carry on a mean-field decoupling of the t-t' Hubbard model. Consider the ansatz where $\phi_i - \phi_j = \pi$, with i and j labeling any two adjacent lattice sites. Except for this difference of π between the phases of the order parameter on two adjacent sites, the phases $\phi_i \equiv \phi$ are site independent and assume any value in $[0, 2\pi]$. The normal state Hamiltonian in RAFT [5, 6, 7] is

$$H \approx \sum_{\mathbf{k} \in RBZ} \Psi_{\mathbf{k}}^\dagger \mathcal{H} \Psi_{\mathbf{k}} + NUQ^2 - NUn^2, \tag{2}$$

where N is the number of sites, and $n = \langle n_{i,\sigma} \rangle$ is the expectation value of the number operator. Because of antiferromagnetic correlations the lattice consists of two sublattices A and B, even though there is no long-range static antiferromagnetic order. The summation runs over the reduced Brillouin zone (RBZ). The Nambu spinor is $\Psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k}\uparrow}^{A\dagger}\ c_{\mathbf{k}\uparrow}^{B\dagger}\ c_{\mathbf{k}\downarrow}^{A\dagger}\ c_{\mathbf{k}\downarrow}^{B\dagger})$, and the Hamiltonian matrix is

$$\mathcal{H} = \begin{pmatrix} -\mu' & \epsilon & Qe^{i\phi} & 0 \\ \epsilon & -\mu' & 0 & -Qe^{i\phi} \\ Qe^{-i\phi} & 0 & -\mu' & \epsilon \\ 0 & -Qe^{-i\phi} & \epsilon & -\mu' \end{pmatrix},$$

yielding the energy spectra $E_\pm(\mathbf{k}) = -\mu'(\mathbf{k}) \pm E_q(\mathbf{k})$, where $\mu'(\mathbf{k}) = \mu - Un + 4t' \cos k_x \cos k_y$, $E_q(\mathbf{k}) = \sqrt{\epsilon^2(\mathbf{k}) + (UQ)^2}$, and $\epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y)$. Because the energy spectra $E_\pm(\mathbf{k})$ do not depend on the phase ϕ one should be able to transform $\mathcal{H}$ to a matrix that does not depend on the phase. This can indeed be done using the spin-dependent gauge transformation $c_{i,\uparrow} \to e^{i\phi/2} c_{i,\uparrow}$ and $c_{i,\downarrow} \to e^{-i\phi/2} c_{i,\downarrow}$. This transformation is equivalent to performing a rotation by angle

$-\phi$ about the z axis for the x and y components of the spin operator. Indeed, upon using this gauge transformation, the spin ladder operators transform according to $S_i^+ \to e^{-i\phi} S_i^+$ and $S_i^- \to e^{i\phi} S_i^-$, which yields:

$$\begin{pmatrix} S_i^x \\ S_i^y \end{pmatrix} \to \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} S_i^x \\ S_i^y \end{pmatrix}.$$

The thermal averages of S_i^x and S_i^y are given by

$$\begin{aligned} \frac{\langle S_i^x \rangle}{\hbar} &= Q\cos\phi, \quad \frac{\langle S_i^y \rangle}{\hbar} = -Q\sin\phi, \quad i \in A, \text{ or} \\ \frac{\langle S_i^x \rangle}{\hbar} &= -Q\cos\phi, \quad \frac{\langle S_i^y \rangle}{\hbar} = Q\sin\phi, \quad i \in B. \end{aligned} \tag{3}$$

Note that $\langle S_i^z \rangle = 0$ for i in both sublattices. Because the phase ϕ assumes any value between 0 and 2π (see below), rotational symmetry will not look broken for times greater than the period of rotation. However if the typical time scale of a probe is much smaller than this period symmetry may appear broken.

2.3. Calculation of the time dependence of phase ϕ

The magnitude Q, which was calculated using the minimization of the mean-field free energy [5, 6, 7], behaves as in a second-order phase transition in agreement with experimental evidence in [4].

Next we calculate the phase using the Heisenberg equation $\frac{dS_j^+}{d\tau} = \frac{1}{i\hbar}[S_j^+, H]$. We consider the limit where electron hopping is neglected in comparison to $\frac{U}{2}(S_j^+ S_j^- + S_j^- S_j^+)$. The limit considered here is $U \sim 3t$-$5t$; this is an intermediate coupling limit where $U > t$ but smaller than the bandwidth $\sim 8t$ when $t' \ll t$. It is justified to use this approximation because spin dynamics is faster than charge dynamics; i.e., an onsite spin flip needs a time $\tau \sim \hbar/U$ to be realized, while a charge hopping between adjacent sites takes a longer time $\tau \sim \hbar/t$, $(U > t)$. In the Heisenberg equation the undecoupled interaction is used instead of RAFT's Hamiltonian (2) in order to treat as best as possible quantum fluctuations. To carry on the calculation, we keep in mind that any site j is on average only partially occupied, and that $|\langle S_j^\pm \rangle| < \hbar/2$. For this reason, terms like $S_j^+ S_j^+ S_j^-$ and $S_j^+ S_j^- S_j^+$ should be kept until the end (these terms normally give zero when acting on a spin up state, but a nonzero contribution is expected when applied to a partially occupied state where thermal averages are meaningful and suitable). In the commutator of the Heisenberg equation $[S_j^+, H] \approx -\frac{U}{2}[S_j^+, (S_j^+ S_j^- + S_j^- S_j^+)]$, we need to calculate $[S_j^+, (S_j^+ S_j^- + S_j^- S_j^+)] = [S_j^+, S_j^+ S_j^-] + [S_j^+, S_j^- S_j^+] = 2\hbar(S_j^+ S_j^z + S_j^z S_j^+)$. Using the fundamental commutation relation $[S_j^z, S_j^+] = \hbar S_j^+$, one gets $S_j^+ S_j^z + S_j^z S_j^+ = \hbar S_j^+ + 2S_j^+ S_j^z$, which leads to

$$\frac{dS_j^+}{d\tau} = iS_j^+ \left(\frac{U}{\hbar} + \frac{2U}{\hbar^2} S_j^z \right), \quad \tau \text{ is time.} \tag{4}$$

Again we stress that this equation is obtained in the intermediate coupling limit (U smaller than the bandwidth but higher than hopping energies), where spin dynamics is not governed by the Heisenberg exchange coupling $\sim t^2/U$ suitable for the strong coupling limit. Eq. (4) gives zero when acting on state $|\uparrow\rangle$ or $|\downarrow\rangle$. However, for a collective state where any site is only partially occupied, one has to take the thermal average of Eq. (4). One then replaces S_i^z by its RAFT's thermal average, which is zero. Integrating Eq. (4) gives for the thermal average

$$\langle S_j^+(\tau) \rangle \approx \langle S_j^+(0) \rangle e^{iU\tau/\hbar}, \tag{5}$$

which yields $\phi = U\tau/\hbar$ modulo 2π when $\langle S_j^+(0) \rangle$ is identified with $|\langle S_j^+(\tau) \rangle|$, $(-|\langle S_j^+(\tau) \rangle|)$, for sublattice A, (B), and $e^{i\phi}$ with $e^{iU\tau/\hbar}$. The angular frequency is thus $\omega_{sf} = U/\hbar$, and period $T_{sf} = 2\pi\hbar/U$ is the time required to perform a spin-flip process, or the time needed for the rotating order parameter $\langle S_i^{x(y)} \rangle$ to complete a 2π revolution in a classical point of view. The magnetic configuration (3) takes on the following form $\langle S_i^x \rangle/\hbar = Q\cos(\omega_{sf}\tau)$, $\langle S_i^y \rangle/\hbar = -Q\sin(\omega_{sf}\tau)$ for i in sublattice A or $\langle S_i^x \rangle/\hbar = -Q\cos(\omega_{sf}\tau)$, $\langle S_i^y \rangle/\hbar = Q\sin(\omega_{sf}\tau)$ for i in sublattice B, and $\langle S_i^z \rangle = 0$ for i in sublattice A or B.

2.4. Interpretation of rotating antiferromagnetism

To illustrate well rotating magnetic order, consider first the much simpler example of the time evolution of a single spin in a magnetic field B along the z-axis, with the initial state given for a spin pointing in the positive x-direction by $|S_x, +\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$. The time-dependent expectation values of the spin components are $\langle S^x \rangle = \frac{\hbar}{2} \cos(\omega t)$, $\langle S^y \rangle = \frac{\hbar}{2} \sin(\omega t)$, and $\langle S^z \rangle = 0$, with $\omega = \frac{|e|B}{m_e c}$. e and m_e are the charge and mass of the electron, respectively, and c is the speed of light. Classically speaking, the spin is confined to rotate about the z-axis in the xy plane with Larmor angular frequency ω. A rotating ferromagnetic state can be realized by placing N such states with the same frequency on a lattice made of N sites. For a rotating antiferromagetic state, opposite initial states ($\pm|S_x, +\rangle$: spins point in opposite directions on the x-axis) are required on each two adjacent sites of the lattice. To relate RAF to spin flip processes, we note that $\langle S^\pm \rangle = \langle S^x \rangle \pm i\langle S^y \rangle = \frac{\hbar}{2} e^{\pm i\omega t}$ in this example. Note that in this example is model independent, which may indicate that all model parameters will do is changing multiplying physical factors, not the physics itself. In a given model, a coupling is necessary for providing the building bloc for RAF, which is the precession of a spin (with no local magnetization) for each lattice site. The RAF state constructed in this way shows a hidden order that can be realized even at finite temperature without violating the Mermin-Wagner theorem [16].

The example above allows us to interpret RAF as a state where spins precess collectively in a synchronized manner in the spins' xy plane around an effective staggered magnetic field $B = m_e c U/\hbar|e|$ caused by onsite Coulomb repulsion. For our many-body system, $\hbar/2$ in $\langle S^\pm \rangle = \frac{\hbar}{2} e^{\pm i\omega t}$ is replaced by the magnitude of the RAF order parameter Q, which can assume values smaller than $1/2$ due to thermal averaging. This state is strongly doping dependent. When doping increases, Q rapidly decreases then vanishes at a doping identified as the quantum critical point underneath the superconducting dome [5, 6, 7, 12, 13, 14]. In comparison to ordinary spin waves in an antiferromagnet, RAF's state could be viewed as a $\mathbf{q} = (\pi, \pi)$ spin wave in an antiferromagnet with zero magnetization. Note however that for our system (where $\langle S_i^z \rangle = 0$), spin-wave theory is not applicable because the spin-wave theory is built around a stable nonzero $\langle S_i^z \rangle$ state.

3. conclusion

The rotating antiferromagnetism theory and Heisenberg equation are combined in order to calculate the phase of the rotating order parameter. This phase behaves linearly in time. This allows us to interpret rotating antiferromagnetism in terms of a Larmor-like spin precession about an effective magnetic field, which is proportional to onsite Coulomb repulsion. Another way to see rotating antiferromagnetism is as an unusual spin-wave at $\mathbf{q} = (\pi, \pi)$ around a zero magnetization. This work was necessary for unveiling the nature of rotating antiferromagnetism, which has been proposed for explaining the pseudogap behavior in high-T_C materials. Rotating antiferromagnetic order is an example of hidden order, which is a serious candidate for the PG state in HTSCs. This is supported by the good success of the rotating antiferromagnetism theory in the calculation of thermodynamics [5, 6, 7], optical conductivity [12, 15], Raman [13], and angle-resolved photoemission spectroscopy properties [14].

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